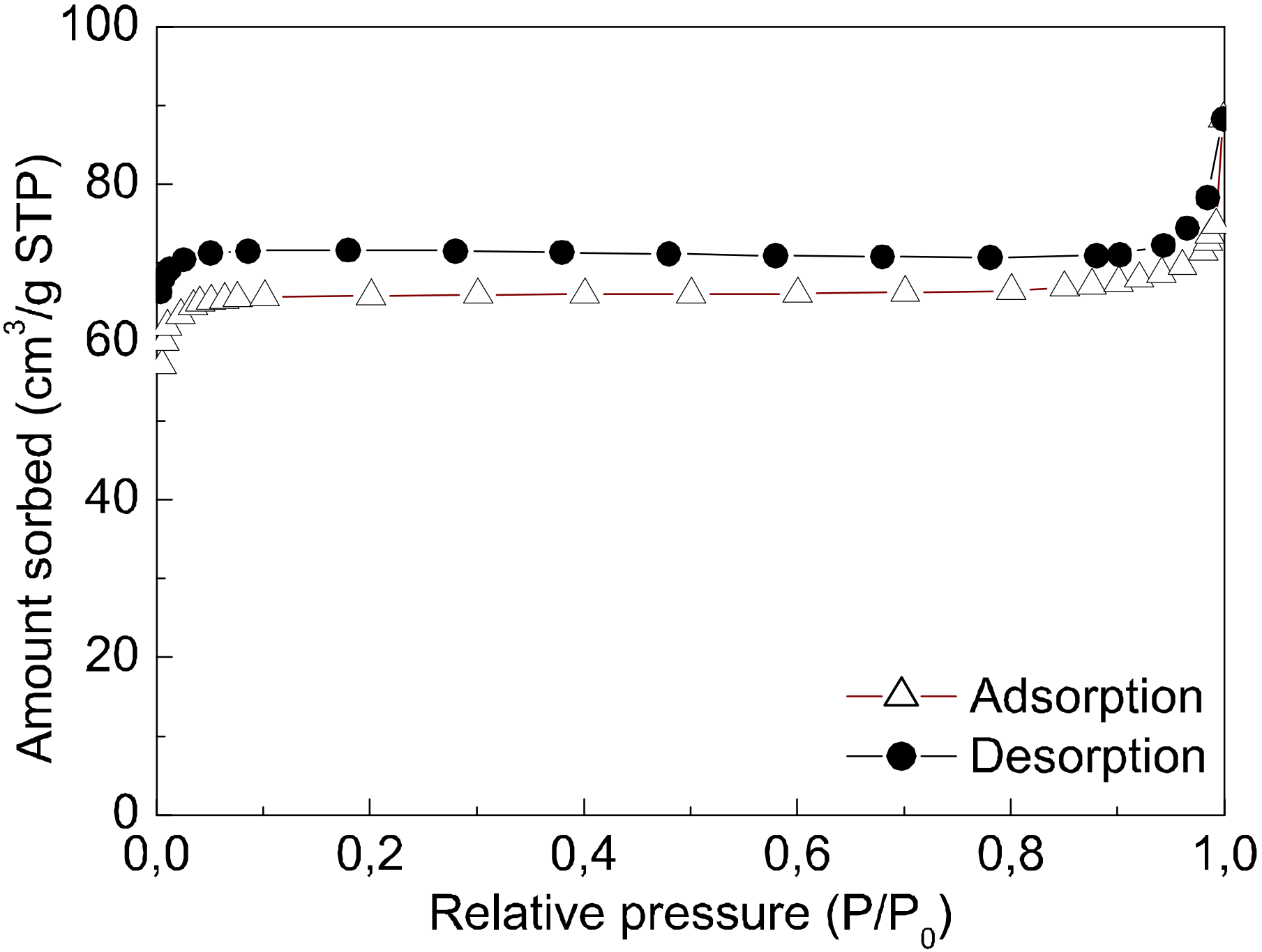
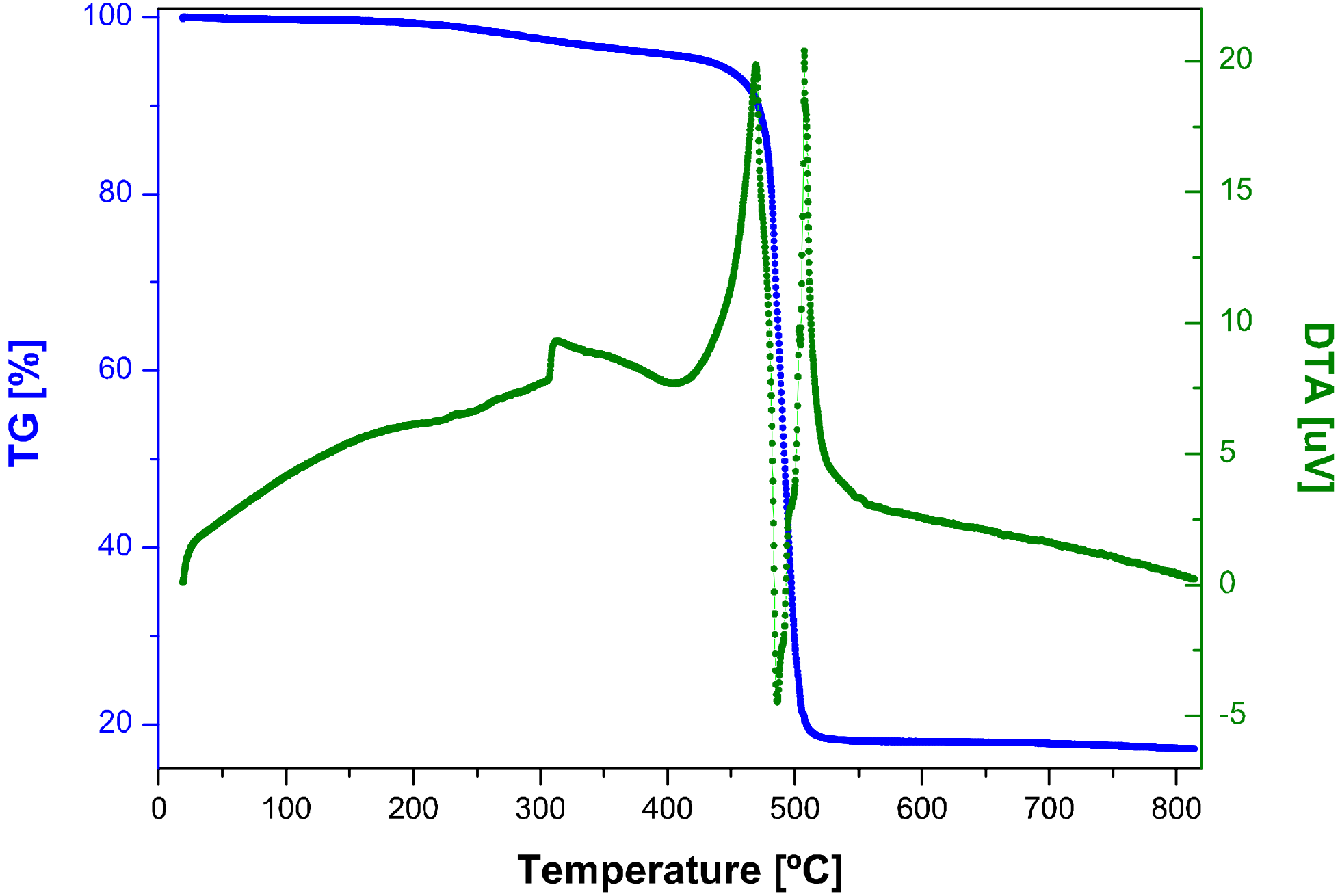
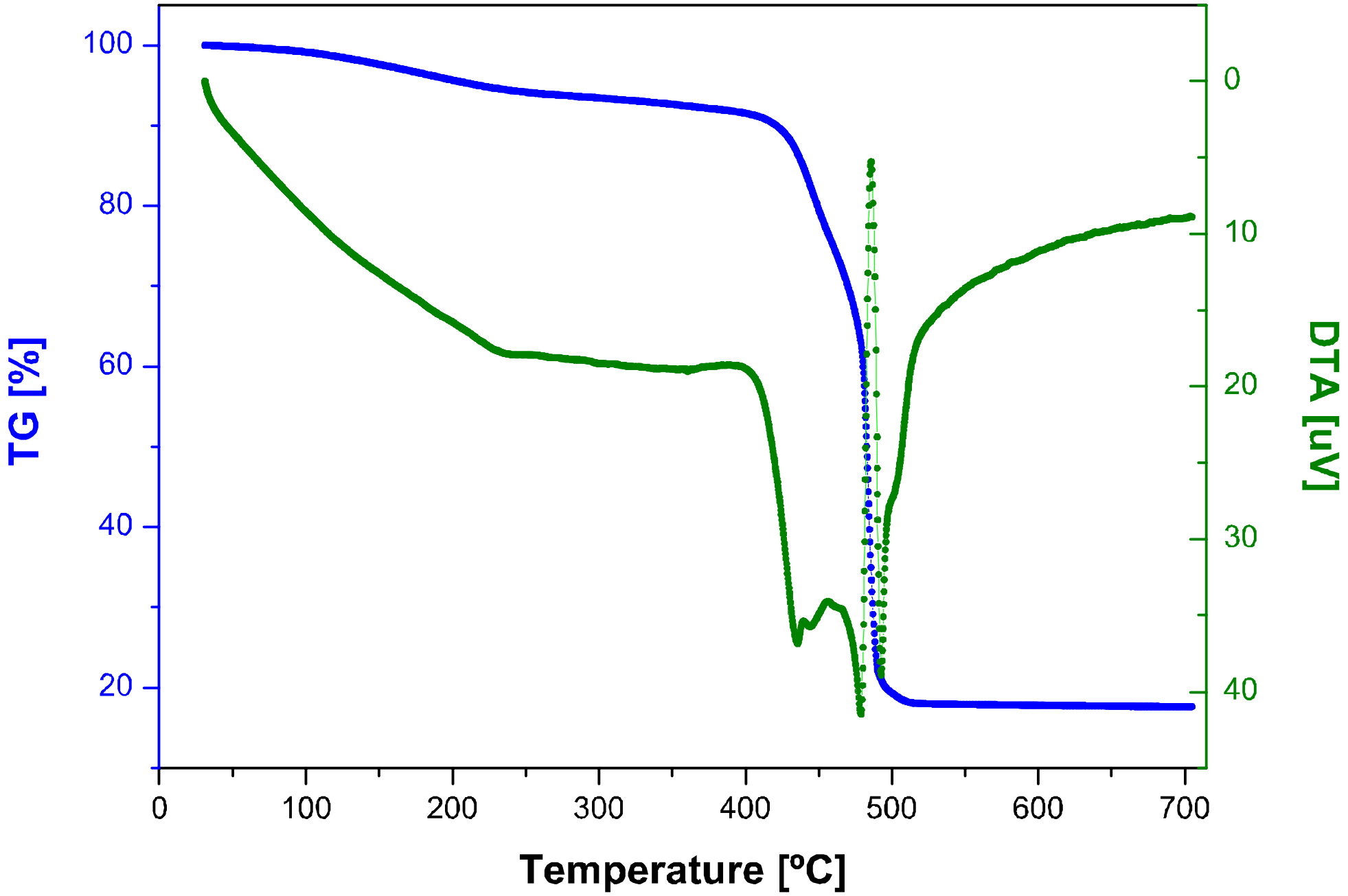

100
80
60
40
20
0
Amount sorbed (cm3/g STP)
0,0
0,2
0,4
0,6
0,8
1,0
Relative pressure (P/P0)
Adsorption
Desorption


100
80
60
40
20
TG [%]
20
15
10
5
0
-5
DTA [uV]
0
100
200
300
400
500
600
700
800
Temperature [ºC]


TG [%]
100
80
60
40
20
DTA [uV]
0
10
20
30
40
0
100
200
300
400
500
600
700
Temperature [ºC]

Supplementary Material (ESI) for Chemical Communications
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space group is P6422.

The net is CHIRAL and a NEW UNINODAL 4-connected

cell parameters for edges of lenght = 1.
a = 3.09730, b = 3.09730, c = 0.74283
alpha = 90.0000, beta = 90.0000, gamma = 120.0000
node positions
0.12479 0.56240 0.83333
Edges:
0.12479 0.56240 0.83333 <-> 0.43760 0.56240 1.16667
0.12479 0.56240 0.83333 <-> -0.12479 0.43760 1.83333

Coordination for X

X 1 -0.1248 0.4376 -0.1667 (0 1-1) 1.000A
X 1 -0.1248 0.4376 1.8333 (0 1 1) 1.000A
X 1 0.4376 0.8752 0.5000 (0 1-1) 1.000A
X 1 0.4376 0.5624 1.1667 (1 1 0) 1.000A

Coordination sequences

X: 1 2 3 4 5 6 7 8 9 10
Num 4 12 30 57 96 150 204 267 348 431
Cum 4 16 46 103 199 349 553 820 1168 1599

Vertex symbol

X Schlafli symbol:{6^5;8}
With circuits:[6.6.6.6.6(2).8(13)]
With rings: [6.6.6.6.6(2).8(11)]

Total Schlafli symbol: {6^5;8}

The ideal net present edges crossing at 1/2,1/2,2/3
that is avoided in the real embedding with flexible ligands that
bend over, avoiding the crossing

classification done with TOPOS :
V. A. Blatov, A. P. Shevchenko and V. N. Serezhkin, J. Appl. Crystallogr., 2000, 33, 1193.
V. A. Blatov, L. Carlucci, G. Ciani and D. M. Proserpio CrystEngComm, 2004, 6(65), 377-395

and optimization done with SYSTRE :
O.Delgado Friedrichs, M. O'Keeffe, Acta Cryst., 2003, A59, 351
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